

CONTINUOUS-TIME QUANTUM WALKS AND TRAPPING

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Recent findings suggest that processes such as the electronic energy transfer through the photosynthetic antenna display quantal features, aspects known from the dynamics of charge carriers along polymer backbones. Hence, in modeling energy transfer one has to leave the classical, master-equation-type formalism and advance towards an increasingly quantum-mechanical picture, while still retaining a local description of the complex network of molecules involved in the transport, say through a tight-binding approach.

Interestingly, the continuous time random walk (CTRW) picture, widely employed in describing transport in random environments, can be mathematically reformulated to yield a quantum-mechanical Hamiltonian of tight-binding type; the procedure uses the mathematical analogies between time-evolution operators in statistical and in quantum mechanics: The result are continuous-time quantum walks (CTQWs). However, beyond these formal analogies, CTRWs and CTQWs display vastly different physical properties. In particular, here we focus on trapping processes on a ring and show, both analytically and numerically, that distinct configurations of traps (ranging from periodical to random) yield strongly different behaviours for the quantal mean survival probability, while classically (under ordered conditions) we always find an exponential decay at long times.

Keywords: Quantum Walks; Random Walks; Exciton transport; Trapping; Perturbation theory.

I. INTRODUCTION

The transport properties of excitons in organic as well as in inorganic molecular solids are of fundamental interest [Kempe, 2003; Woerner *et al.*, 2004; Mülken *et al.*, 2006; Sillanpää *et al.*, 2007; Olaya-Castro *et al.*, 2008; Zhou *et al.*, 2008]. In general, at high temperatures the transport is incoherent and can be efficiently modeled by continuous-time random walks (CTRWs) over sets of participating centers (atoms, molecules, etc.) [Montroll & Weiss, 1965]. In this case the transport follows a master equation. The transfer rates between the participating centers can be related to the spatial arrangement of the centers. The arrangement is captured by the so-called Laplacian Matrix \mathbf{L} which we will identify here with the transfer matrix of the CTRW. However, when dealing with quantum particles at low densities and low temperatures, decoherence can be suppressed to a large extent: The study of transport in this regime requires different modeling tools, able to mimic the coherent features. Clearly, quantum mechanical transport phenomena follow Schrödinger's equation. In order to make contact to CTRW we relate the Hamiltonian of the system to the classical transfer matrix, $\mathbf{H} = -\mathbf{L}$; this yields a description mathematically closely connected to the classical master equation approach. Indeed, this realizes a quantum mechanical analog of the CTRWs defined on a discrete structure, i.e. the so-called continuous-time quantum walks (CTQWs). However, apart from formal analogies, coherence can give rise to very peculiar properties (e.g. Anderson localization [Anderson, 1958], crucial dependences of the transport on the starting position [Mülken *et al.*, 2006] and a quadratic speed-up of the chemical distance covered [Agliari *et al.*, 2008]) with

no counterpart in classical transport. These effects allow interesting and cross-disciplinary applications and can also be exploited in experiments in order to distinguish whether the transport is rather classical or rather quantum mechanical [Mülken *et al.*, 2007].

In particular, a common means for probing the transport relies on the interaction with other species, such as impurity atoms or molecules (found in or doped into the medium) which irreversibly trap the charges or quench the excitations. Consequently, a great deal of recent theoretical work has focused on investigating essential features of basic trapping models, wherein a single particle moves in a medium containing different arrangements of traps. Indeed, much is known about the decay when the motion is incoherent [Van Kampen, 1981; Blumen *et al.*, 1983; 1986; ben-Avraham & Havlin, 2000], while (as we will show here) when quantum effects become important, strong deviations from the classical results occur.

In a set of early works the dynamics of coherent excitations on a chain with randomly distributed traps has been investigated using several methods [Hemenger *et al.*, 1974; Kenkre, 1978; Huber, 1980; Parris, 1991] which provided a reasonably description of the process at short times and in the asymptotic limit. On the other hand, from the experimental point of view, the most relevant regime is the one of intermediate times; in this time interval some striking effects have been recently highlighted [Mülken *et al.*, 2007; Mülken *et al.*, 2008].

Here we focus on trapping processes taking place on a finite ring where the traps are distributed according to different arrangements: the traps are either gathered in a cluster or distributed periodically or randomly. In these cases the classical survival probability $P_M(t)$ has been studied intensively (see e.g. [ben-Avraham & Havlin

2000]). In fact, under ordered conditions $P_M(t)$ is known to exponentially decay to zero. Conversely, for a random distribution of traps $P_M(t)$ exhibits different time regimes: At long times it follows a stretched exponential which turns into a pure exponential when finite size effects dominate. As for the CTQW, the emergence of intrinsic quantum-mechanical effects, such as tunneling, prevents the decomposition of the problem into a collection of disconnected intervals and, as we will see, the mean survival probability $\Pi_M(t)$ is strongly affected by the trap arrangement. Hence, by following the temporal decay of $\Pi_M(t)$ we can extract information about the geometry. Furthermore, we show that in the cases analyzed here $P_M(t)$ and $\Pi_M(t)$ exhibit qualitatively different behaviours; this allows to determine the nature, either rather coherent or rather incoherent, of the transport process.

Our paper is structured as follows: In Sec. II we provide a brief summary of the main concepts and of the formulae concerning CTQWs. In Sec. III we introduce a mathematical formalism useful for analyzing trapping in the CTQW picture. In the following Sec. IV, we consider special arrangements of traps on a ring and we investigate the mean survival probability by means of a perturbative approach; these analytical findings are corroborated by numerical results. In Sec. V we study the case of random distributions of traps and finally, in Sec. VI we present our comments and conclusions.

II. CONTINUOUS TIME QUANTUM WALK

Let us consider a graph \mathcal{G} made up of N nodes and algebraically described by the so-called adjacency matrix \mathbf{A} : The non-diagonal elements A_{ij} equal 1 if nodes i and j are connected by a bond and 0 otherwise; the diagonal elements A_{ii} are 0. From the adjacency matrix we can directly derive some interesting quantities concerning the corresponding graph. For instance the coordination number of a node i is $z_i = \sum_j A_{ij}$ and the number of walks of length ℓ from i to j is given by $(A^\ell)_{ij}$ [Biggs, 1974].

We also define the Laplacian operator \mathbf{L} according to $L_{ij} = z_i \delta_{ij} - A_{ij}$; the set of all N eigenvalues of L is called the Laplacian spectrum of \mathcal{G} . Interestingly, the Laplacian spectrum is intimately related not only to dynamical processes involving particles moving on the graph, but also to dynamical processes involving the network itself; these include energy transfer and diffusion-reaction processes as well as the relaxation of polymer networks, just to name a few (see for example [Mohar, 1991; Galiceanu & Blumen, 2007] and references therein).

In the context of coherent and incoherent transport it is worth underlining that, being symmetric and non-negative definite, \mathbf{L} can generate both a probability conserving Markov process and a unitary process [Childs & Goldstone, 2004; Mülken & Blumen, 2005; Volta *et al.*, 2006].

Now, continuous-time random walks (CTRWs) [Montroll & Weiss, 1965] are described by the following Master Equation:

$$\frac{d}{dt} p_{k,j}(t) = \sum_{l=1}^N T_{kl} p_{l,j}(t), \quad (1)$$

being $p_{k,j}(t)$ the conditional probability that the walker is on node k when it started from node j at time 0. If the walk is unbiased the transmission rates γ are bond-independent and the transfer matrix \mathbf{T} is related to the Laplacian operator through $\mathbf{T} = -\gamma \mathbf{L}$ (in the following we set $\gamma = 1$).

We now define the quantum-mechanical analog of the CTRW, i.e. the CTQW, by identifying the Hamiltonian of the system with the classical transfer matrix, $\mathbf{H} = -\mathbf{T}$ [Farhi & Gutmann, 1998; Mülken & Blumen, 2005]. Hence, given the orthonormal basis set $|j\rangle$, representing the walker localized at the node j , we can write

$$\mathbf{H} = \sum_{j=1}^N z_j |j\rangle\langle j| - \sum_{j=1}^N \sum_{k \in \text{NN}j} |k\rangle\langle j|, \quad (2)$$

where in the second sum k runs over all nearest neighbors (NN) of j . The operator in Eq. 2 is also known as tight-binding Hamiltonian. Actually, the choice of the Hamiltonian \mathbf{H} is, in general, not unique [Childs & Goldstone, 2004] and Eq. 2 has two important advantages: It allows to take into account the local properties of the arbitrary substrate and, remarkably, it yields a mathematical formulation displaying important analogies with the classical picture. In fact, the dynamics of the CTQW can be described by the transition amplitude $\alpha_{k,j}(t)$ from state $|j\rangle$ to state $|k\rangle$, which obeys the following Schrödinger equation:

$$\frac{d}{dt} \alpha_{k,j}(t) = -i \sum_{l=1}^N H_{kl} \alpha_{l,j}(t), \quad (3)$$

structurally very similar to Eq. 1. The solution of Eq. 3 can be formally written as

$$\alpha_{k,j}(t) = \langle k | \exp(-i\mathbf{H}t) | j \rangle, \quad (4)$$

whose squared magnitude provides the quantum mechanical transition probability $\pi_{k,j}(t) \equiv |\alpha_{k,j}(t)|^2$.

In general, it is convenient to introduce the orthonormal basis $|\Phi_n\rangle$, $n \in [1, N]$ which diagonalizes \mathbf{H} ; the correspondent set of eigenvalues is denoted by $\{E_n\}_{n=1,\dots,N}$. Thus, we can write

$$\pi_{k,j}(t) = \left| \sum_{n=1}^N \langle k | e^{-iE_n t} | \Phi_n \rangle \langle \Phi_n | j \rangle \right|^2. \quad (5)$$

It should be underlined that while both problems (CTRW and CTQW) are linear, and thus many results

obtained in solving CTRWs (eigenvalues and eigenfunctions) can be readily reutilized for CTQWs, the physically relevant properties of the two cases differ vastly: Thus, in the absence of traps CTQWs are symmetric under time-inversion, which precludes them from attaining equipartition for the $\pi_{k,j}(t)$ (such as the $p_{k,j}(t)$ for CTRWs) at long times. Also, the quantal system keeps memory of the initial conditions, exemplified by the occurrence of quasi-revivals [Mülken & Blumen, 2005; Mülken & Blumen, 2006].

III. CTQWS IN THE PRESENCE OF TRAPS

As discussed in the previous section, the operators describing the dynamics of CTQWs and of CTRWs share the same set of eigenvalues and of eigenstates. However, when new contributions (arising e.g. from the interaction with external fields or absorbing sites) are incorporated, the eigenvalues and the eigestates start to differ. In the following we introduce a formalism useful to analyze the dynamics of CTQWs and CTRWs in the presence of traps; for this we will denote with \mathbf{H}_0 and \mathbf{T}_0 the unperturbed operators without traps.

Let us consider a system where M out of the N nodes are traps; we label the trap positions with m_j , with $j = 1, \dots, M$, and we denote this set with \mathcal{M} .

For substitutional traps the system can be described by the following effective (but non-Hermitian) Hamiltonian [Mülken *et al.*, 2007]

$$\mathbf{H} = \mathbf{H}_0 - i\mathbf{\Gamma}, \quad (6)$$

where $\mathbf{\Gamma}$ is the trapping operator defined as

$$\mathbf{\Gamma} = \sum_{j=1}^M \Gamma_{m_j} |m_j\rangle\langle m_j|. \quad (7)$$

The capture strength Γ_{m_j} determines the rate of decay for a particle located at trap site m_j ; here we will take the Γ_{m_j} to be equal for all traps, i.e. $\Gamma_{m_j} \equiv \Gamma$ for all j . The limit $\Gamma \rightarrow \infty$ corresponds to perfect traps, which means that a classical particle is immediately absorbed when reaching any trap.

Due to the non-hermiticity of \mathbf{H} , its eigenvalues are complex and can be written as $E_l = \epsilon_l - i\gamma_l$ ($l = 1, \dots, N$); moreover, the set of its left and right eigenvectors, $|\Phi_l\rangle$ and $\langle\tilde{\Phi}_l|$, respectively, can be chosen to be biorthonormal ($\langle\tilde{\Phi}_l|\Phi_{l'}\rangle = \delta_{l,l'}$) and to satisfy the completeness relation $\sum_{l=1}^N |\Phi_l\rangle\langle\tilde{\Phi}_l| = \mathbf{1}$. Therefore, according to Eq. 3, the transition amplitude can be evaluated as

$$\alpha_{k,j}(t) = \sum_{l=1}^N e^{-(\gamma_l + i\epsilon_l)t} \langle k|\Phi_l\rangle \langle\tilde{\Phi}_l|j\rangle, \quad (8)$$

from which $\pi_{k,j}(t) = |\alpha_{k,j}(t)|^2$ follows.

Of particular interest, due to its relation to experimental observables, is the mean survival probability $\Pi_M(t)$ which can be expressed as [Mülken *et al.*, 2007]

$$\begin{aligned} \Pi_M &\equiv \frac{1}{N-M} \sum_{j \notin \mathcal{M}} \sum_{k \notin \mathcal{M}} \pi_{kj}(t) \\ &= \frac{1}{N-M} \sum_{l=1}^N e^{-2\gamma_l t} \left(1 - 2 \sum_{m \in \mathcal{M}} \langle\tilde{\Phi}_l|m\rangle \langle m|\Phi_l\rangle \right) \\ &\quad + \frac{1}{N-M} \sum_{l,l'=1}^N e^{-i(E_l - E_{l'})} \left(\sum_{m \in \mathcal{M}} \langle\tilde{\Phi}_{l'}|m\rangle \langle m|\Phi_l\rangle \right)^2 \end{aligned} \quad (9)$$

The temporal decay of $\Pi_M(t)$ is determined by the imaginary parts of E_l , i.e. by the γ_l . As shown in [Mülken *et al.*, 2007] at intermediate and long times and for $M \ll N$ the $\Pi_M(t)$ can be approximated by a sum of exponentially decaying terms:

$$\Pi_M \approx \frac{1}{N-M} \sum_{l=1}^N e^{-2\gamma_l t}, \quad (10)$$

and is dominated asymptotically by the smallest γ_l values.

Now, in the incoherent, classical transport case trapping is incorporated into the CTRW according to

$$\mathbf{T} = \mathbf{T}_0 - \mathbf{\Gamma} = -\mathbf{L} - \mathbf{\Gamma}. \quad (11)$$

The transfer operator \mathbf{T} is therefore real and symmetric, and it leads to real, strictly negative eigenvalues which we denote by $-\lambda_l$; to them correspond the eigenstates $|\phi_l\rangle$.

Analogously, the mean survival probability for the CTRW can be written as

$$\begin{aligned} P_M(t) &\equiv \sum_{j \notin \mathcal{M}} \sum_{k \notin \mathcal{M}} p_{kj}(t) \\ &= \frac{1}{N-M} \sum_{l=1}^N e^{-\lambda_l t} \left| \sum_{k \notin \mathcal{M}} \langle k|\phi_l\rangle \right|^2. \end{aligned} \quad (12)$$

From Eq. 12 one may deduce that $P_M(t)$ attains in general rather quickly an exponential form; furthermore, if the smallest eigenvalue λ_{\min} is well separated from the next closest eigenvalue, $P_M(t)$ is dominated by λ_{\min} and by the corresponding eigenstate $|\phi_{\min}\rangle$ [Mülken *et al.*, 2007; Mülken *et al.*, 2008]:

$$P_M(t) \approx \frac{1}{N-M} e^{-\lambda_{\min} t} \left| \sum_{k \notin \mathcal{M}} \langle k|\phi_{\min}\rangle \right|^2. \quad (13)$$

Lower estimates of the gap Δ between the two smallest eigenvalues have been found in the past for special choices of operators (see e.g. [Chen M., 1997] and references therein). For instance, the operator \mathbf{T}_0 has $\lambda_{\min} = 0$; its next smallest eigenvalue represents the algebraic connectivity of the graph, namely the relative number of

edges needed to be deleted to generate a bipartition. In the case of a k -regular graph Δ is bounded from below by $k/(DN)$, being D the diameter of the graph, i.e. the maximum distance between any two vertices [Chung F.R.K., 1996].

IV. PERTURBATIVE APPROACH FOR TRAPPING ON A RING

When the strength Γ of the trap is small with respect to the couplings between neighbouring nodes (which here means $\Gamma \ll 1$), we can treat the effective Hamiltonian introduced in Eq. 6 along the lines of time-independent perturbation theory.

Before developing this strategy we fix the structure \mathcal{G} , by considering a ring of length N so that the coordination number equals 2 for all sites ($\mathbf{Z} = 2\mathbf{I}$), where we assume N to be even. For the corresponding Hamiltonian \mathbf{H}_0 we know exactly all the eigenvalues and eigenvectors; one has namely

$$E_l^{(0)} = 2 - 2\cos(2\pi l/N) \quad (14)$$

and

$$|\Phi_l^{(0)}\rangle = \frac{1}{\sqrt{N}} \sum_{j=1}^N e^{-i2\pi lj/N} |j\rangle. \quad (15)$$

We underline that all the eigenvalues, apart from $E_{N/2} = 4$ and $E_N = 0$, are two-fold degenerate, $E_l = E_{N-l}$ ($l = 1, 2, \dots, N/2 - 1$). We now apply perturbation theory to evaluate to first order the corrections $E_l^{(1)}$ to the eigenvalues E_l . For $l = N/2$ and for $l = N$ we use the non-degenerate expression

$$E_l^{(1)} = -i\Gamma \sum_{m \in \mathcal{M}} \left| \langle m | \Phi_l^{(0)} \rangle \right|^2 \quad (16)$$

and get

$$E_{N/2} = 4 - i\Gamma \frac{M}{N} \quad \text{and} \quad E_N = -i\Gamma \frac{M}{N}. \quad (17)$$

For l different from $N/2$ and N we set

$$V_{i,j} \equiv \langle \Phi_i^{(0)} | -i\Gamma | \Phi_j^{(0)} \rangle \quad (18)$$

and we apply the expression valid for two-fold degenerate solutions of \mathbf{H}_0 :

$$E_l^{(1)} = \frac{1}{2} (V_{l,l} + V_{N-l,N-l}) \pm \frac{1}{2} \left[(V_{l,l} - V_{N-l,N-l})^2 + 4|V_{l,N-l}|^2 \right]^{1/2}, \quad (19)$$

where we choose the positive sign for $l \in [1, N/2 - 1]$ and the negative sign for $l \in [N/2 + 1, N - 1]$. Now we have

$$V_{l,l} \equiv V_{N-l,N-l} = -i\Gamma \frac{M}{N}, \quad (20)$$

independently of the trap arrangement and

$$\begin{aligned} V_{l,N-l} &= -i\Gamma/N \sum_{j=1}^M \exp\{2i\pi m_j[l - (N-l)]/N\} \\ &= -i\Gamma/N \sum_{j=1}^M \exp(4i\pi l m_j/N). \end{aligned} \quad (21)$$

By inserting the last results into Eq. 19 we get

$$E_l^{(1)} = \frac{-i\Gamma}{N} \left(M \pm \left| \sum_{j=1}^M e^{2i\pi 2l m_j/N} \right| \right). \quad (22)$$

We notice that for special trap arrangements the $E_l^{(1)}$ can be calculated exactly: The most striking results are obtained when the exponential in the sum in Eq. 22 equals one of the values from the set $\{1, i, -1, -i\}$. Then the absolute value of the sum reduces to $|\sum_{j=1}^M \exp(i4\pi l m_j/N)| = M$. For this there have to exist indices $l \neq N/2$ and $l \neq N$ such that m_j can be expressed as

$$m_j = \frac{N}{8l}(4k_j + r) + c \quad (23)$$

where k_j and c are arbitrary integers and $r = 0, 1, 2$ or 3 , corresponding to $1, i, -1$ or $-i$, respectively. Consequently, we obtain for the correction

$$E_l^{(1)} = -i\Gamma \frac{M}{N} \quad \text{and} \quad E_{N-l}^{(1)} = 0, \quad (24)$$

so that the degeneracy is always lifted.

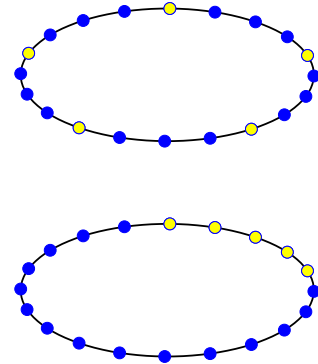


FIG. 1: Examples of periodic (top) and sequential (bottom) arrangements of $M = 5$ traps on a ring of size $N = 20$.

Let us now focus on a periodic distribution of traps with $m_j = jN/M$, while $N/M \in \mathbb{N}$. It is easy to see that in this case there exists a non-empty set Υ of distinct values of $l \in [1, N/2 - 1]$ satisfying the condition of Eq. 23; this occurs for $2l/M \in \mathbb{N}$, so that the cardinality of Υ is given by the number of integers in $\{2l/M\}_{l=1,2,\dots,N/2-1}$, namely by

$$|\Upsilon| = \begin{cases} \lfloor (N-2)/M \rfloor & \text{for even } M, \\ \lfloor (N-2)/2M \rfloor & \text{for odd } M, \end{cases} \quad (25)$$

where $\lfloor x \rfloor$ denotes the largest integer less than or equal to x . In particular, for both $M = 1$ and $M = 2$ we have $|\Upsilon| = N/2 - 1$. Now, the numerical diagonalization of the Hamiltonian \mathbf{H} shows that for $l \in \Upsilon$ we get $\gamma_{N-l} = 0$ (not only in first order in Γ). Consequently, the corresponding term in Eq. 9 decays to a non vanishing value, and from Eq. 10 we have for $t \rightarrow \infty$:

$$\Pi_M(t) \approx \frac{|\Upsilon|}{N - M}. \quad (26)$$

Hence, recalling Eq. 25, for large structures with $M \ll N$, $\Pi_M(t)$ asymptotically decays to $1/M$ (even case) and to $1/(2M)$ (odd case). Figure 2 shows results obtained for a ring of size $N = 300$ with a periodic arrangement of $M = 10$ ($|\Upsilon| = 29$) and $M = 75$ ($|\Upsilon| = 1$) traps. Consequently, the survival probability $\Pi_M(t)$ decays to the constant values $1/10$ and $1/225$, respectively. From a physical point of view, the finite limit for the survival probability stems from the existence of stationary states to which the nodes in \mathcal{M} do not contribute, so that they never “see” the traps. This genuine quantum-mechanical effect has no counterpart in the classical case where, for finite structures, the survival probability always decays to zero in the presence of traps. In particular, as shown in Fig. 2, $P_M(t)$ decays exponentially, as expected.

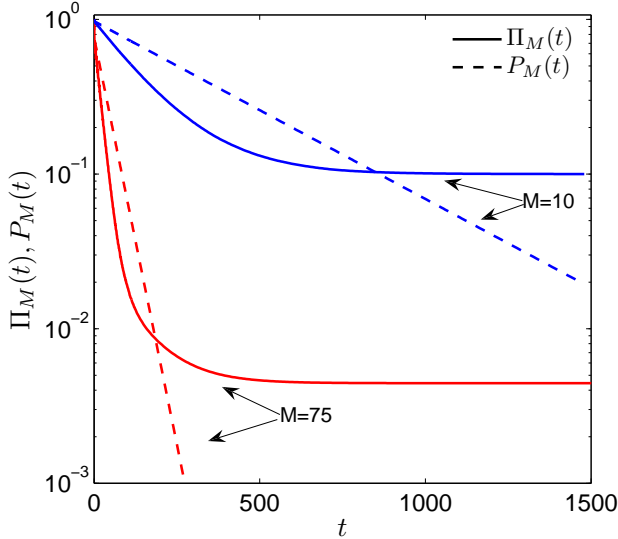


FIG. 2: Survival probabilities $\Pi_M(t)$ (continuous line) and $P_M(t)$ (dotted lines) on a ring of size $N = 300$ and $\Gamma = 0.01$ in the presence of $M = 10$ and of $M = 75$ traps arranged periodically, i.e. $m_j = jN/M$. Note the semilogarithmic scales.

Let us now focus on another special configuration of M traps, $M > 1$: we consider a sequential arrangement, such that $m_j = j$ and $j = 1, \dots, M$. Hence, Eq. 21 can

be written as

$$\begin{aligned} V_{l,N-l} &= -i\Gamma/N \sum_{j=1}^M \exp(4i\pi jl/N) \\ &= \frac{-i\Gamma}{N} \frac{\exp(4i\pi lM/N) - 1}{\exp(4i\pi il/N) - 1} \exp(4i\pi il/N) \\ &= \frac{-i\Gamma}{N} \frac{\sin(2\pi lM/N)}{\sin(2\pi l/N)} \exp[2i\pi l(M+1)/N], \end{aligned} \quad (27)$$

from which we get

$$E_l^{(1)} = \frac{-i\Gamma}{N} \left(M \pm \frac{\sin(2\pi lM/N)}{\sin(2\pi l/N)} \right). \quad (28)$$

We notice that since $l \neq N/2$ and $l \neq N$ then $2l/N \notin \mathbb{N}$, while for $2lM/N \in \mathbb{N}$ then $E_l^{(1)} = E_{N-l}^{(1)} = -i\Gamma M/N$. In particular, when $M = N/2$, we have $\gamma_l = M/N$ for each value of $l \in [1, N]$. As a result, in Eq. 9 the first term vanishes due to the completeness property and the fact that the γ_l are no longer l -dependent. As for the second term, by neglecting oscillations, we get

$$\Pi_M(t) \approx \frac{M}{N-M} e^{-2\Gamma t M/N} = \frac{1}{2} e^{-\Gamma t}, \quad (29)$$

which is independent of N . As shown in Fig. 3 the exponential behaviour predicted by Eq. 29 holds also for intermediate times.

In Fig. 4 we compare the survival probabilities of CTQWs and CTRWs: as highlighted by the semi-logarithmic plot, the decay is exponential in both cases, although faster in the former. Indeed, for the CTRWs we have in the long-time limit from Eq. 12:

$$P_M(t) \approx \frac{N-M}{N} e^{-\Gamma M t/N} = \frac{1}{2} e^{-\Gamma t/2}, \quad (30)$$

where we used the fact that the smallest eigenvalue is $\Gamma M/N$. By comparing Eq. 29 and Eq. 30 we see that, although the decay is exponential in both cases, the decay rate is twice larger for $\Pi_M(t)$ than for $P_M(t)$.

V. RANDOM DISTRIBUTIONS OF TRAPS

We now take N to be odd (so as not to fulfill Eq. 23) and consider random arrangements of traps: we pick M distinct trap locations randomly from a uniform distribution and determine the corresponding $\Pi_M(t)$ and $P_M(t)$. Then we average these over different, independent realizations to determine $\langle \Pi_M(t) \rangle$ and $\langle P_M(t) \rangle$. As already mentioned in Sec. I, $\langle P_M(t) \rangle$ exhibits different behaviours: in an infinite system the decay law is a stretched exponential at long times, whereas in finite systems at such times the decay gets to be exponential. In Fig. 5 we show evidence of the long-time exponential behaviour of $\langle P_M(t) \rangle$ in systems of relatively small size.

Let us now consider $\langle \Pi_M(t) \rangle$ for random trap arrangements. Now, the $\langle \Pi_M(t) \rangle$ decay differs qualitatively from

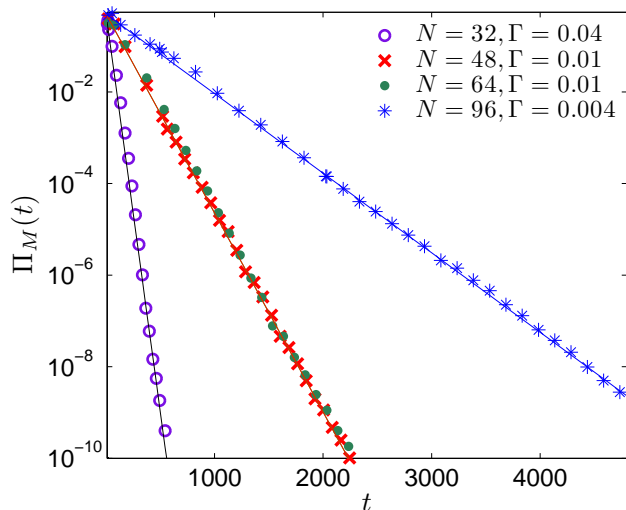


FIG. 3: Survival probability $\Pi_M(t)$ on rings of size $N = 32, 48, 64$ and 96 for $\Gamma = 0.04, 0.01, 0.004$, as indicated. The number of traps is $M = N/2$ and they are placed consecutively, i.e. $m_j = j$. The straight lines represent Eq. 29.

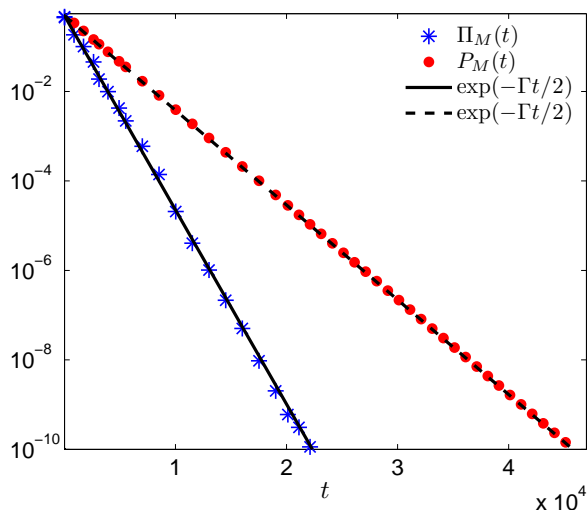


FIG. 4: Survival probabilities $\Pi_M(t)$ and $P_M(t)$ on rings of size $N = 48$ for $\Gamma = 0.001$; the number of traps is $M = N/2$ and they are placed consecutively, i.e. $m_j = j$. The straight lines represent Eq. 29 (continuous line) and Eq. 30 (dashed line).

that of the $\Pi_M(t)$ analyzed in the previous section. As shown in Fig. 6, for intermediate times the average survival probability displays a power law, which decays more slowly than exponentially:

$$\langle \Pi_M(t) \rangle \sim t^{-1/\mu}. \quad (31)$$

A similar result has already been obtained for CTQWs on a finite chain with two traps at its ends ($\mathcal{M} = \{1, N\}$), in the presence of either nearest-neighbour [Mülken *et al.*, 2007] or long-range interactions [Mülken *et al.*, 2008].

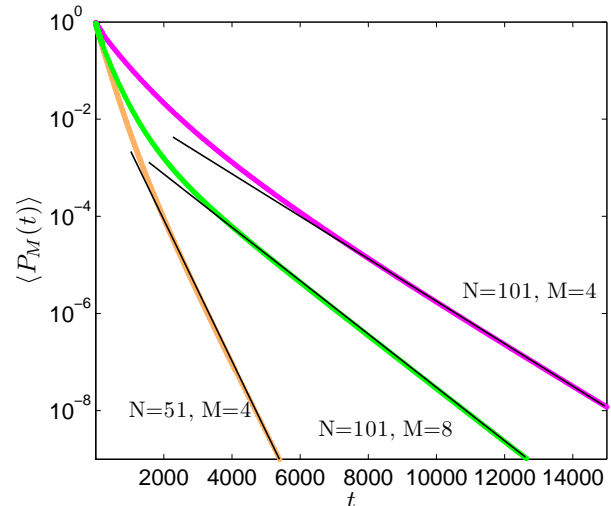


FIG. 5: Average survival probabilities $\langle P_M(t) \rangle$ for rings of sizes $N = 51$ and 101 . Here $\Gamma = 0.1$ and M is either 4 or 8 . The data presented have been averaged over 120 different realizations, see text. The straight lines highlight the exponential decay.

There one could understand the power law decay based on the imaginary part of the Hamiltonian spectrum $\{\gamma_l\}$, which in a large interval scales algebraically with l . By fitting the numerical data obtained for different sizes and concentrations we get the characteristic exponent μ depicted in the inset of Fig. 6.

VI. CONCLUSIONS

In conclusion, we have modeled the coherent dynamics by continuous-time quantum walks and studied interactions with traps: Taking a periodic chain as substrate, we calculated the mean quantal survival probability $\Pi_M(t)$ and we compared it to the classical $P_M(t)$ for different trap arrangements. The quantum problem was approached both analytically (by means of perturbative theory) and numerically, showing that the spatial distribution of the traps significantly affects $\Pi_M(t)$. In particular, when the traps are arranged periodically throughout the substrate, $\Pi_M(t)$ decays asymptotically to a nonvanishing value which depends directly on the system size N and on the number of traps M (e.g., when $M = 2$, $\Pi_2(t) \rightarrow 1/2$ for $t \rightarrow \infty$). This is a genuine quantum-mechanical effect with no counterpart in classical mechanics, where $P_M(t)$ decays to zero for finite systems.

Another interesting, deterministic trap configuration is realized by distributing the traps consecutively such to form a cluster; then at intermediate and long times the survival probability decays exponentially with the characteristic time Γ^{-1} . Now, for the same trap configuration, the characteristic time for the classical survival

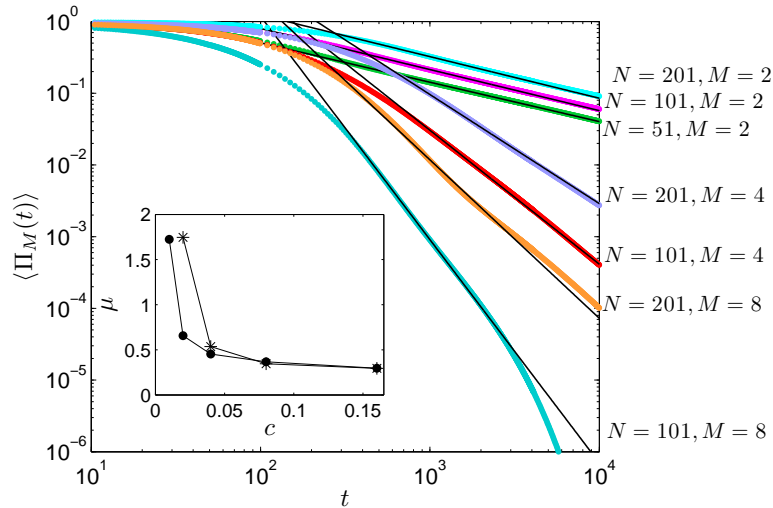


FIG. 6: $\langle \Pi_M(t) \rangle$ and μ for rings of sizes $N = 51, 101$, and 201 . Here $\Gamma = 0.1$ and M is $2, 4$, or 8 , as indicated. The data presented have been averaged over 120 different realizations. The main figure displays the average survival probabilities $\langle \Pi_M(t) \rangle$ in double logarithmic scales. The straight lines represent the best fit. The inset displays the exponent μ as a function of $c = M/N$ for systems of sizes $N = 201$ (*) and $N = 101$ (•).

probability doubles, being $2\Gamma^{-1}$.

When the traps are distributed randomly on the substrate, a further, qualitatively different behaviour of $\Pi_M(t)$ is obtained. In fact, by averaging over different independent configurations we find in this case that at intermediate times $\langle \Pi_M(t) \rangle$ decays algebraically, i.e. $\langle \Pi_M(t) \rangle \sim t^{-1/\mu}$, where μ depends on M and N and is related to the imaginary part of the Hamiltonian spectrum. On the other hand, for systems of relatively small size we find that in the same time range finite-size effects dominate $\langle \Pi_M(t) \rangle$, giving rise to an exponential decay.

These results establish that studying the decay due to trapping is indeed an advantageous means to monitor the system's evolution, as it allows to determine the nature of the transport, which can be either rather coherent or rather incoherent. Moreover, the behaviour exhibited by $\Pi_M(t)$, being qualitatively affected by the trap configurations, may be used to distinguish between these.

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